(Chloromethyl)trimethylsilane at 160 K

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Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(Si–C) = 0.004 Å
R factor = 0.040
wR factor = 0.115
Data-to-parameter ratio = 23.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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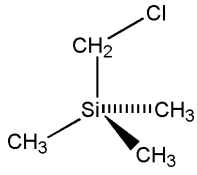
(Chloromethyl)trimethylsilane, Me_3SiCH_2Cl or $C_4H_{11}ClSi$, is a liquid at room temperature, and it was crystallized using *in situ* methods. The C—Si—C bond angles involving the chloromethyl group are somewhat smaller than those involving only methyl groups [105.5 (2)–109.47 (19)° *versus* 110.01 (19)–111.2 (2)°], which is ascribable to both the electronegative and the steric effects of the Cl atom.

Comment

(Chloromethyl)trimethylsilane, (I), is a liquid under ambient conditions, and a crystal was obtained by *in situ* crystallization of a sample held in a hand-drawn Pyrex capillary (Boese & Nussbaumer, 1994).



(I)

Molecules of (I) adopt the expected tetrahedral configuration at Si (Fig. 1). Si—C bond distances fall into the range 1.848 (4)–1.880 (4) Å, although to within experimental error the bond distances and angles have C_s symmetry, with a mirror plane passing through atoms Si1, C1, Cl1 and C4; the C4—Si1—C1—Cl1 torsion angle [175.3 (2)°] shows a somewhat more significant deviation from the symmetry. The bond angles at atom Si1 involving the more electronegative CH_2Cl group are smaller [105.5 (2)–109.47 (19)°] than those involving only methyl groups [110.01 (19)–111.2 (2)°]. The smaller

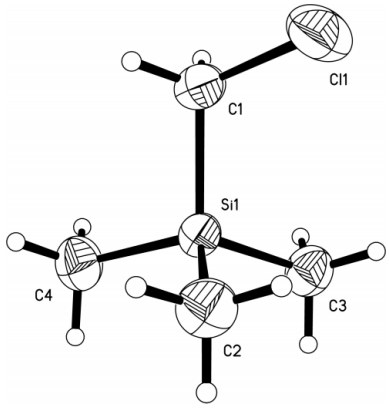


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented as spheres of arbitrary radii.

magnitude of C1—Si1—C4 [105.5 (2)°] relative to C1—Si1—C2 [109.4 (2)°] and C1—Si1—C3 [109.47 (19)°] presumably reflects the steric influence of the Cl atom.

The only intermolecular interactions falling within the sum of the van der Waals radii (Bondi, 1964) of the participating atoms are weak Cl1···H33^{i} [symmetry code (i): $-x, -y, z-\frac{1}{2}$] interactions (2.93 Å; the sum of the van der Waals radii of Cl and H is 2.95 Å). These result in chains that spiral about the 2_1 axis parallel to the *c* direction (Fig. 2).

Experimental

A sample of (I) was obtained from Aldrich and used as received. Compound (I) is a liquid under ambient conditions and it was crystallized *in situ* in a capillary (o.d. 0.34 mm) mounted on the diffractometer. A crystal was grown by first establishing a seed in a small volume of the liquid at 182.8 K, and then cooling at a rate of 10 K h^{-1}. The sample was then cooled to 160 K for data collection.

Crystal data

$C_4H_{11}ClSi$
M_r = 122.67
Orthorhombic, $Pna2_1$
a = 13.8776 (13) Å
b = 6.3855 (9) Å
c = 8.4000 (10) Å
V = 744.37 (15) Å^3
Z = 4
D_x = 1.095 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 72 reflections
θ = 15–16°
μ = 0.56 mm^{-1}
T = 160 K
Cylinder, colourless
0.50 × 0.39 × 0.39 mm
0.50 mm length, 0.39 mm radius

Data collection

Stoe STADI-4 diffractometer equipped with an Oxford Cryosystems low-temperature device (Cosier & Glazer, 1986)
ω–θ scans
Absorption correction: ψ scan [azimuthal absorption correction (North *et al.*, 1968) applied using *XPREP* (Sheldrick, 1997)]
T_{min} = 0.741, T_{max} = 0.804
3768 measured reflections
1306 independent reflections
1186 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°
$h = -1 \rightarrow 16$
$k = -7 \rightarrow 7$
$l = -9 \rightarrow 9$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.02
1305 reflections
56 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F)^2 + (0.0706P)^2 + 0.41P]$ where $P = 0.3333\max(0,F_o^2) + 0.6667F_c^2$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 602 Friedel pairs
Flack parameter = −0.17 (17)

Table 1
Selected geometric parameters (Å, °).

Cl1—C1	1.798 (5)	Si1—C3	1.862 (4)
Si1—C1	1.880 (4)	Si1—C4	1.867 (4)
Si1—C2	1.848 (4)		
C1—Si1—C2	109.4 (2)	C2—Si1—C4	111.2 (2)
C1—Si1—C3	109.47 (19)	C3—Si1—C4	111.18 (19)
C1—Si1—C4	105.5 (2)	Cl1—C1—Si1	111.9 (2)
C2—Si1—C3	110.01 (19)		

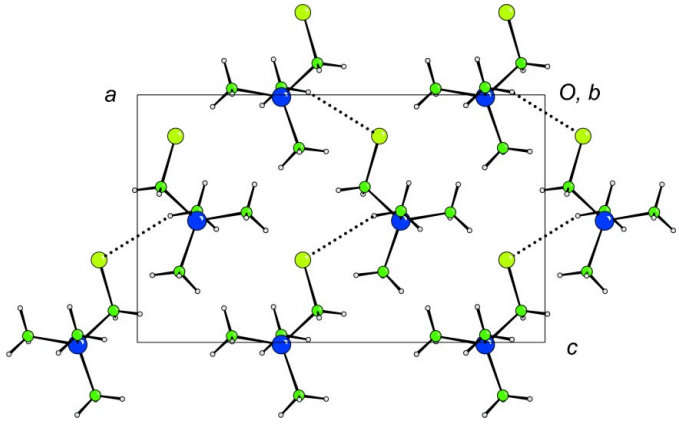


Figure 2
The molecular packing of (I), viewed along the *b* axis. Weak intermolecular Cl1···H33 interactions are shown as dotted lines.

The positions of the H atoms were recalculated geometrically after each refinement cycle, using a C—H distance of 1.00 Å, and they were assigned U_{iso}(H) = 1.2U_{eq}(C). The 10,1,0 reflection was omitted as an outlier.

Data collection: *DIF*4 (Stoe & Cie, 1990); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1990); program(s) used to solve structure: *DIRDIF* (Beurskens *et al.*, 1996); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996) and *XP* (Sheldrick, 1997); software used to prepare material for publication: *CRYSTALS*, *enCIFer* (CCDC, 2003) and *PLATON* (Spek, 2003) used within *WinGX* (Farrugia, 1999).

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References

Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, C. K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Beurskens, P. T., Admiraal, G., Beurskens, G., Bosman, W. P., García-Granda, S., Gould, R. O., Smits, J. M. M. & Smykalla, C. (1996). *The DIRDIF96 Program System*. Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
Boese, R. & Nussbaumer, M. (1994). *Correlations, Transformations and Interactions in Organic Crystal Chemistry*, *IUCr Crystallographic Symposia*, Vol. 7, edited by D. W. Jones & A. Katrusiak, pp. 20–37. Oxford University Press.
Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.
CCDC (2003). *enCIFer*. Test version. Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, England.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *XP*, *XPREP* and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1990). *DIF*4 (Version 7.09/DOS) and *REDU*4 (Version 7.03/DOS). Stoe & Cie, Darmstadt, Germany.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.